AMENDMENTS TO THE CLAIMS

This listing of claims represents a complete listing of the claims and replaces all other versions of claims in this application:

1. (currently amended) A method of calculating an intermolecular interaction energy between two molecules, comprising the steps of:

providing a first molecule;

decomposing the molecule into two or more molecular fragments; ~~and~~

introducing one or more pairs of ~~conjugated~~ caps having a first cap member and a second cap member at each decomposition point in the molecular fragment ~~at one or more locations in the molecule~~ to create a plurality of molecular portions, wherein each molecular portion comprises a fragment of the first molecule and at least one cap member; ~~of the first and second cap members of at least one pair of conjugated caps~~

coupling each pair of caps to form one or more conjugated caps;

determining the interaction energies (a) between each molecular portion and the second molecule, and (b) between each pair of conjugated caps and the second molecule;

calculating an intermolecular interaction energy between the first molecule and a second molecule based on the interaction energy determinations; and

displaying the results of the calculated intermolecular interaction energy.

2. (currently amended) The method as set forth in claim 1, wherein the ~~providing step comprises electronically generating the~~ first molecule is provided by electronically generating a representation of a physical molecule.

3. (currently amended) The method as set forth in claim 2, wherein the decomposing step comprises electronically cutting the representation of the molecule.

4. (currently amended) The method as set forth in claim 3, wherein the introducing step comprises electronically introducing the one or more pairs of ~~conjugated~~ caps into the electronically generated first molecule.

5-6 (cancelled).

7. (currently amended) The method as set forth in claim 1 ~~claim 6~~, wherein the ~~calculating~~ step of determining interaction energy between the molecular portion and the second molecule comprises ~~at least one first computing system~~ calculating an interaction energy between a first molecular portion and the second molecule on a first computing system, and ~~a second computing system~~ calculating the interaction energy between a second molecular portion and the second molecule on a second computing system.

8. (currently amended) The method as set forth in claim 1 ~~claim 6~~, wherein the calculating step comprises ~~further comprising the step of~~

summing together the interaction energies determined for each of the molecular portions and the second molecule to provide a total interaction energy of the molecular portions.

9. (currently amended) The method as set forth in claim 8, wherein the calculating step comprises ~~further comprising the step of~~

summing together the ~~one or more~~ conjugated cap interaction energies determined ~~obtained~~ from each pair ~~of the one or more pairs~~ of conjugated caps and the second molecule to provide a total conjugated cap interaction energy; and

subtracting the total conjugated cap interaction energy from the total interaction energy of the molecular portions ~~to provide an intermolecular interaction energy between the first molecule and the second molecule~~.

10. (original) The method as set forth in claim 9, wherein the intermolecular interaction energy is a quantum mechanical intermolecular interaction energy.

11. (original) The method as set forth in claim 1, wherein the first molecule is a polyatomic species.

12. (original) The method as set forth in claim 11, wherein the polyatomic species is selected from the group consisting of a material, a protein, a peptide, a polymer, DNA, and RNA.

13. (original) The method as set forth in claim 1, wherein the second molecule is selected from the group consisting of an ion, a water molecule, an inorganic molecule, an organic molecule, a drug molecule, and a biological molecule.

14. (original) The method as set forth in claim 1, wherein the first molecule is a protein or a peptide and the second molecule is a drug molecule.

15. (original) The method as set forth in claim 1, wherein the first and second cap members are independently selected from the group consisting of NH_2, HNCOH, CH_3, CRH_2, CRHCOH, $CRHCONH_2$, $CRHNH_2$, CRHNHCOH, COH, and $CONH_2$, wherein R is a carbon-containing group.

16. (currently amended) A computer-readable medium having stored thereon instructions for calculating an intermolecular interaction energy, said instructions comprising:

instructions for providing a first molecule;

instructions for decomposing the first molecule into two or more molecular fragments; ~~and~~

instructions for introducing one or more pairs of ~~conjugated~~ caps having a first cap member and a second cap member at each decomposition point in the molecular fragment ~~at one or more locations in the molecule~~ to create a plurality of molecular portions, wherein each molecular portion comprises a fragment of the first molecule and at least one cap member; ~~of the first and second cap members of at least one pair of conjugated caps~~

instructions for coupling each pair of caps to form one or more conjugated caps;

instructions for determining the interaction energies (a) between each molecular portion and the second molecule, and (b) between each pair of conjugated caps and the second molecule;

instructions for calculating an intermolecular interaction energy between the first molecule and a second molecule based on the interaction energy determinations; and

instructions for displaying the results of the calculated intermolecular interaction energy; wherein the computer-readable medium is a physical medium.

17-19.

20. (currently amended) The medium as set forth in claim 16, wherein the instructions for calculating an intermolecular interaction energy comprise ~~claim 18, further comprising~~

instructions for summing together the interaction energies determined for each of the molecular portions and the second molecule to provide a total interaction energy of the molecular portions.

21. (currently amended) The medium as set forth in claim 20, wherein the instructions for calculating an intermolecular interaction energy comprise ~~further comprising~~

instructions for summing together the ~~one or more~~ conjugated cap interaction energies determined ~~obtained~~ from each pair ~~of the one or more pairs~~ of conjugated caps and the second molecule to calculate a total conjugated cap interaction energy; and

instructions for subtracting the total conjugated cap interaction energy from the total interaction energy of the molecular portions to calculate the ~~provide an~~ intermolecular interaction energy between the first molecule and the second molecule.

22. (original) The medium as set forth in claim 21, wherein the intermolecular interaction energy is a quantum mechanical intermolecular interaction energy.

23. (original) The medium as set forth in claim 16, wherein the first molecule is a polyatomic species.

24. (currently amended) The medium as set forth in claim 23 ~~claim 19~~, wherein the polyatomic species is selected from the group consisting of a material, a protein, a peptide, a polymer, DNA, and RNA.

25. (currently amended) The medium as set forth in claim 16 ~~claim 17~~, wherein the second molecule is selected from the group consisting of an ion, a water molecule, an inorganic molecule, an organic molecule, a drug molecule, and a biological molecule.

26. (original) The medium as set forth in claim 16, wherein the first and second cap members are selected from the group consisting of NH_2, HNCOH, CH_3, CRH_2, CRHCOH, $CRHCONH_2$, $CRHNH_2$, CRHNHCOH, COH, and $CONH_2$, wherein R is a carbon-containing group.

27. (currently amended) A computer system for calculating an intermolecular interaction energy, the system comprising:

a molecular generation module that provides a first molecule;

a molecular decomposition module that decomposes the molecule into two or more molecular fragments; and

a molecular cap introduction module that introduces one or more pairs of ~~conjugated~~ caps having a first cap member and a second cap member at each decomposition point in the molecular fragment ~~at one or more locations in the first molecule~~ to create a plurality of molecular portions, wherein each molecular portion comprises a fragment of the first molecule and at least one cap member; ~~one of the first and second cap members of at least one pair of conjugated caps~~

a coupling module that couples each pair of caps to form one or more conjugated caps;

an interaction energy module that determines the interaction energies (a) between each molecular portion and the second molecule, and (b) between each pair of conjugated caps and the second molecule;

an intermolecular interaction energy module that calculates an intermolecular interaction energy between the first molecule and a second molecule based on the interaction energy determinations; and

a displaying module that displays the results of the calculated intermolecular interaction energy.

28-29. (cancelled).

30. (currently amended) The system as set forth in claim 27 ~~claim 29~~, wherein the interaction energy ~~calculation~~ module comprises at least one first computing system that determines ~~calculates~~ an interaction energy between a first molecular portion and the second molecule, and at least one second computing system that determines ~~calculates~~ an interaction energy between a second molecular portion and the second molecule.

31. (currently amended) The system as set forth in claim 27 ~~claim 29~~, wherein the intermolecular interaction energy ~~calculation~~ module sums together the interaction energies determined for each of the molecular portions and the second molecule to provide a total interaction energy of the molecular portions.

32. (currently amended) The system as set forth in claim 31, wherein the ~~molecular~~ intermolecular interaction energy module

sums together the ~~one or more~~ conjugated cap interaction energies determined ~~obtained~~ from each pair ~~of the one or more pairs~~ of conjugated caps and the second molecule to provide a total conjugated cap interaction energy; and

subtracts the total conjugated cap interaction energy from the total interaction energy of the molecular portions to ~~provide an~~ calculate the intermolecular interaction energy between the first molecule and the second molecule.

33. (original) The system as set forth in claim 32, wherein the intermolecular interaction energy is a quantum mechanical intermolecular interaction energy.

34. (original) The system as set forth in claim 27, wherein the first molecule is a polyatomic species.

35. (original) The system as set forth in claim 34, wherein the polyatomic species is selected from the group consisting of a material, a protein, a peptide, a polymer, DNA, and RNA.

36. (original) The system as set forth in claim 27, wherein the second molecule is selected from the group consisting of an ion, a water molecule, an inorganic molecule, an organic molecule, a drug molecule, and a biological molecule.

37. (original) The system as set forth in claim 27, wherein the first molecule is a protein or a peptide and the second molecule is water.

38. (original) The system as set forth in claim 27, wherein the first and second cap members are selected from the group consisting of NH_2, HNCOH, CH_3, CRH_2, CRHCOH, $CRHCONH_2$, $CRHNH_2$, CRHNHCOH, COH, and $CONH_2$, wherein R is a carbon-containing group.

39. (withdrawn) A composition comprising:

a molecule comprising a plurality of units, and

a plurality of pairs of conjugated caps having a first cap member and a second cap member, wherein each of the plurality of pairs of conjugated caps is inserted between two of the plurality of units under conditions effective to substantially preserve the properties of a chemical bond being cut to insert the pair of conjugated caps and wherein the first cap member substantially mimics the electronic effect of the units of the molecule on a first side of the pair of conjugated caps and the second cap member substantially mimics the electronic effect of the units of the molecule on a second side of the pair of conjugated caps.

40. (withdrawn) The composition as set forth in claim 39, wherein the pairs of conjugated caps form molecular species.

41. (withdrawn) The composition as set forth in claim 39, where the molecule comprises two or more units.

42. (withdrawn) The composition as set forth in claim 39, wherein the molecule is selected from the group consisting of a protein, a peptide, a polymer, DNA, and RNA.

43. (withdrawn) The composition as set forth in claim 39, wherein the first and second cap members are selected from the group consisting of NH_2, HNCOH, CH_3, CRH_2, CRHCOH, $CRHCONH_2$, $CRHNH_2$, CRHNHCOH, COH, and $CONH_2$, wherein R is a carbon-containing group.

44. (withdrawn) The composition as set forth in claim 39, wherein at least two of the molecular fragments in the molecule are fused together through the molecular caps.